Indian J. Phys. **65B** (5), 427-430 (1991)

Dynamics of proteins

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Abstract: A dynamical model has been suggested to explain successfully the observed sudden sharp fall in the Lamb-Mössbauer factor above a characteristic temperature, $T_r \sim 210$ K, in metmyoglobin protein crystal. The sudden increase in the mean square displacement of the Mössbauer nucleus ^{57}Fe, located at the biologically active site in the macromolecule, above T_r is essentially due to the release of additional degrees of freedom which come about because of the onset of, hitherto absent, vibrations of atoms surrounding it. Similar results follow for other proteins.

Keywords: Protein structure, Mössbauer effect in proteins, biological macromolecules.

PACS No: 87.15. He

1. Introduction

Recent studies of biological macromolecules using a variety of probes indicate that the functional activity in such a molecule is related intimately to its molecular dynamic aspects (Berg *et al* 1979a, 1979b, Albanese *et al* 1984). Proteins constitute an important class of biological macromolecules and so far, a few of them—myoglobin, metmyoglobin, deoxymyoglobin and ferritin have been studied for their temperature dependent dynamical behaviour using X-ray scattering and Mössbauer radiation absorption spectroscopy. However, these studies have been performed using crystal of proteins and not in *in-vivo* situation to avoid extreme complications which such a study would entail. Nevertheless, a common feature of proteins which emerges from these studies is that there is a sudden change in their dynamical behaviour at a certain characteristic temperature, T_r, which is not too high (~ 200 K). Such a behaviour is not there in an ordinary molecular crystal. It is, therefore, important to understand the peculiar dynamical behaviour of proteins. In the present study, we consider the case of metmyoglobin.

Parak *et al* (1981) have reported the result of their measurements of Lamb-Mössbauer factor, f on polycrystalline metmyoglobin in the temperature range 4.2-293 K using nuclear gamma resonance absorption experiment. Their measurements clearly show a sudden sharp increase in the mean square displace-

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ment, MSD, of ^{57}Fe, which is at the biologically active site, at temperature ~ 210 K. No broadening of the Mössbauer line was observed indicating the absence of diffusive motion of ^{57}Fe nucleus at the characteristic temperature and above. A few theoretical models (Shaitan and Rubin 1980, Kilyachkov *et al* 1980, Parak *et al* 1981, 1982, Frauenfelder *et al* 1979) have been suggested to explain the sudden fall in f above the characteristic temperature. However, each one of them yields the values of the physical parameters, occurring therein, which are not realistic. For instance, in one of the models, the mass of the molecule which moves rigidly with the Mössbauer nuclei turns out to be $\sim$ 100 a.m.u. (Shaitan and Rubin 1980). We suggest an alternative theoretical model to explain the observed temperature dependent MSD and hence f of ^{57}Fe in metmyoglobin.

2. Mathematical formalism

Lamb-Mössbauer recoiless factor, f, in the Mössbauer absorption experiment is given as follows :

$$f=\exp(-k^2 \langle u_i^2(0, 0) \rangle_T) \tag{1}$$

where $\hbar\,|\,\underline{k}\,|$ is the magnitude of momentum of the Mössbauer radiation and $\langle u_i^2(0, 0) \rangle_T$ is the temperature dependent displacement auto-correlation function of the Mössbauer nucleus in the i-th direction ($i=x$, y or z). The angular bracket implies the quantum-mechanical expectation value as well as the thermal averaging of $u_i^2(0, 0)$.

In the case of proteins, for temperatures above T_r the displacement $\underline{u}(0, 0)$ of the Mössbauer nucleus from its equilibrium position takes the following form :

$$\underline{u}(0, 0)=\underline{u}_t(0, 0)+\underline{u}_a(0, 0) \tag{2}$$

where $\underline{u}_t(0, 0)$ is the displacement due to translational modes and $\underline{u}_a(0, 0)$ is the displacement due to the additional modes which set in just above T_r.

Assuming that there is no coupling between the 't' and 'a' modes and evaluating the total auto correlation function, $\langle u^2(0, 0) \rangle_T$, we get :

$$\langle u^2(0, 0) \rangle_T=\langle u_t^2(0, 0) \rangle_T+\langle u_a^2(0, 0) \rangle_T \tag{3}$$

Using eq. (3), expression (1) becomes

$$f=f_t.f_a \tag{4}$$

3. Results and discussion

Calculations have been performed to determine the temperature dependent MSD of ^{57}Fe in metmyoglobin crystal in the temperature range 0-300 K. For temperatures less than T_r, we find that the Debye distribution function of phonons with characteristic Debye temperature $\theta_D=160$ K is able to reproduce reasonably well the observed MSD (Parak *et al* 1981) as shown in Figure 1. These modes

continue to exist at higher temperatures also and therefore to determine $\langle u_a^2(0,0)\rangle_T$ for any temperature $T > T_r$, the contribution of $\langle u_t^2(0,0)\rangle_T$ has been subtracted from the total observed MSD. $\langle u_a^2(0,0)\rangle_T$ increases sharply with increase in temperature upto the maximum temperature 293 K and therefore one cannot use any simple model to reproduce these. However, we find that it is possible to explain $\langle u_a^2(0,0)\rangle_T$ if we allow the number of additional degrees of freedom that result above T_r to be temperature dependent. Indeed, we find that if we consider the additional modes to be characterized by an Einstein temperature equal to 86 K and

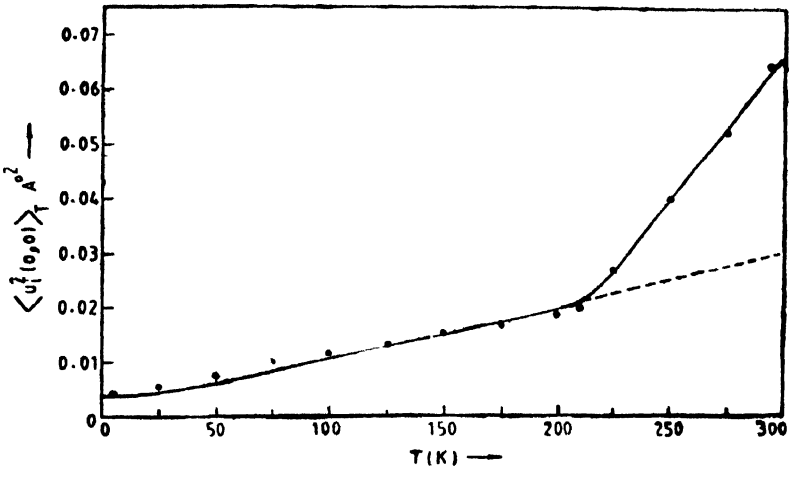

Figure 1. Comparison of calculated values of MSD of ^{57}Fe in metmyoglobin protein crystal in the temperature range 0-300 K with the experimental results of Parak *et al* (1981). ○ denote the experimental points and —— represent the present calculations.

vary the number of degrees of freedom from zero at 210 K, ~ 15% at 225 K, ~ 51% at 250 K, ~ 77% at 275 and ~ 100% at 293 K, we are able to reproduce the observed experimental values of $\langle u_a^2(0,0)\rangle_T$. This implies that as T_r is reached, the dynamical behaviour of ^{57}Fe changes because the atoms around it start vibrating giving rise to an increase in its MSD. With increase in temperature, atoms further away from the ^{57}Fe also start participating in the process. Thus, the biological activity keeps spreading to more and more particles as the temperature is raised. Similar results follow for other proteins as well.

4. Conclusion

From our study we conclude that it is possible to relate the sudden sharp increase in MSD above the temperature T_r of ^{57}Fe in metmyoglobin crystal to additional number of degrees of freedom which result from the onset of, hitherto absent, vibrations of particles of proteins surrounding it.

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